

## **Thermodynamic, elastic, and vibrational (IR/Raman) behavior of mixed type-AB carbonated hydroxylapatite by density functional theory**

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### **ABSTRACT**

The present investigation reports the equation of state, thermodynamic, and thermoelastic properties of type AB carbonated apatite [CAp-AB,  $\text{Ca}_{10}(\text{CO}_3)^B(\text{PO}_4)_5(\text{CO}_3)^A$ , space group *P1*], as obtained from density functional theory simulations and the quasi-harmonic approximation. The static (0 K) third-order Birch-Murnaghan equation of state resulted in the parameters  $K_0 = 104.3(8)$  GPa,  $K' = 4.3(1)$ , and  $V_0 = 517.9(2)$  Å<sup>3</sup>, whereas at room temperature (300 K) they were  $K_T = 101.98$  GPa,  $K' = 4.12$ , and  $V_0 = 524.486$  GPa. Thermodynamics and thermoelasticity were calculated in the temperature range 0–800 K and between 0 and 30 GPa.

Furthermore, the dependence of the infrared/Raman spectra of type-AB carbonated apatite with pressure is also reported, which could be useful for researchers interested in vibrational spectroscopy. The theoretical results corroborate the few experimental ones on a similar type-AB carbonated hydroxylapatite and provide further details over wide pressure and temperature ranges on the elastic, thermodynamic, and infrared/Raman properties of this important mineral found in both geological and biological environments.

**Keywords:** Type-AB carbonated apatite, thermodynamic properties, elastic properties, density functional theory, quasi-harmonic approximation